INL Researchers Revamp Nuclear Simulations

Place a uranium fuel rod in a nuclear reactor, and all sorts of interesting things start to happen. Once self-sustaining nuclear fission begins, the resultant chain reaction causes uranium atoms to decay into xenon, krypton and other elements that zip around the fuel, knocking atoms loose from the fuel's ordered, crystalline structure. Fractures, cracks and voids form. Air bubbles created during the manufacturing process migrate around the hot fuel and join together to form larger pockets.

Nuclear engineers expect these natural processes to occur, changing how fuel conducts heat and responds to stress over its lifetime. Through decades of engineering and experimental analysis, nuclear scientists have developed a number of simple computer models that describe fuel performance and other reactor behavior. These "legacy" models provide good approximations of what happens in present-day reactors. But Generation IV reactors, candidates for the Global Nuclear Energy Partnership and the Next Generation Nuclear Reactor, will be significantly different. Some will run at high temperatures, demand new materials to handle corrosive coolants, and require passive safety features.

This image illustrates an all-hexahedral element computational mesh of a simplified model of the Advanced Test Reactor at INL. Meshes such as this one support INL's advanced reactor modeling activities that involve collaborations between scientists at INL, Los Alamos National Laboratory and Sandia National Laboratories. Figure is courtesy of Scott Lucas and Glen Hansen, INL, and Steve Owen, Sandia National Laboratories.

"These are reactors that are really going to be very efficient and reliable," says Ronaldo Szilard, who heads the INL Nuclear Science and Engineering Division. "In order to have effective designs, we're going to need new models with much better fidelity."

To facilitate new reactor design, INL researchers are working on creating a new, multiphysics simulation capability that will model a reactor from the scale of atoms to an entire reactor assembly. This effort represents a fundamentally different approach to nuclear simulation, one that will stretch computational physics and capacity. At the end of the road, researchers hope, will be a bottom-up nuclear reactor simulation with improved predictive capabilities, one that can assist in reactor design; improving safety, boosting efficiency and helping researchers anticipate challenges years in advance.

Solving coupled problems

Nuclear reactors are full of physical processes that are difficult for computer scientists to model. Fuel degradation is a prime example. When cracks form in uranium fuel, they change the structure of the fuel rods, affecting how the fuel conducts heat. In turn, the way fuel conducts heat impacts how its structure changes over time.

Although it seems like a chicken-and-egg problem, in nature these two processes work in lockstep; what physicists call "coupling." But traditional approaches have only been able to model such complex, intertwined problems by treating each process separately. Simplifying or removing the coupling between physical processes makes them easier to solve computationally, but it also introduces a number of inaccuracies into simulations, many of which could have significant effects on Generation IV designs. "You lose a lot of important information with existing models," says Szilard. "The challenge here is to fit the entire problem into one simulation instead of solving individual processes independently. To do that, the whole computational process needs to be changed."

Fuel Performance Prediction

Nowadays, understanding the limits and properties of fuel is an expensive experimental process. After manufacturing test fuel, nuclear researchers must place the fuel in a test reactor, remove it to analyze the damage, then repeat the process until the design works as desired. From these experiments, physicists developed quantitative models that describe what to expect as fuel is used up in a reactor. But due to historical computer limitations, these models are restricted to one dimension, and because they depend on experiments, the results are only useful for a specific type of fuel and specific test conditions.

Image: Nuclear fuel can accumulate many types of damage over the course of its lifetime.

Nuclear fuel can accumulate many types of damage over the course of its lifetime, including a) air pockets that merge and migrate to create a void in the center of the fuel and b) buildup of fission products. Images from Donald R. Olander, "Fundamental Aspects of Nuclear Reactor Fuel Elements," TID-26711-P1, National Technical Information Service, U.S. Department of Commerce, Springfield, VA 22161, ISBN 0-87079-031-5 (v.1)

"The old models are strongly based on correlations or empirical models you develop by looking at the data," says INL mathematician Glen Hansen. "The problem is if the new reactor is a fundamentally different design, it's probably not going to behave the same way as the test reactor used to develop that data." To develop next generation nuclear reactors, computer scientists need next generation models: ones that work in three dimensions, are more flexible and reduce the reliance on experiments. "The next step is to go back to the basic equations of physics," Hansen says.

One of the first steps to solving coupled physics problems is to solve them in small chunks. "Although the same physical principles are in effect over an entire reactor, you can't solve that complex system of equations directly on the computer," says Hansen. "You have to break the problem up into little tiny pieces to form a mesh." Hansen's specialty is developing meshes that divide up objects, from fuel cladding to the swirling water that cools a reactor, into smaller areas the computer can model. In a simulation, each area within the fuel mesh, for example, will contain a host of physical information; including temperature, the number of neutrons being created, and structural state. Meshing is an important stage in developing a model that can solve coupled problems like predicting fuel degradation. "A high quality mesh, in conjunction with advanced multiphysics methods, gives you the mathematics needed to couple physics problems together and lets you solve them without losing accuracy," Hansen says. "It's only very recently that we've developed the mathematical methods to solve these complex issues and computers powerful enough to solve them on."

Using meshing and other computational tools, Hansen is working to develop a model that can predict fuel performance over the course of its lifetime. In the long term, he hopes to further enhance his multiphysics approach by adding information on what happens to fuel at the smallest scales.

Down to the atomic level

To develop a truly predictive model of fuel performance, the multiphysics team is partnering with Dieter Wolf and his colleagues in the INL Materials Properties and Performance Department to study how radiation affects nuclear fuel at the atomic scale.

As the first step in building a model of uranium dioxide fuel, physicist Tapan Desai tested how a heated block of millions of uranium and oxygen ions deforms when stretched. On the computer monitor, Desai's simulation is built to approximate what a fuel rod looks like at the atomic level: adjacent patches of differently-oriented crystals. The boundaries between these crystals are the weakest points in a material, the likeliest places for cracks to form. Atoms move rapidly in these spaces, and to a lesser extent within the crystals themselves. When a material is stretched, these rearrangements can have a permanent effect on the structure.

Desai's simulated uranium dioxide behaved much like the actual ceramic does in laboratory tests when stretched at high temperature. Building on these baseline simulations, the team is now working on the next step: colliding fast-moving atoms into the simulated material to study radiation effects. Wolf's team is also working on ways to scale simulations up to the microscopic level and longer time scales.

"These simulations of atomic-level polycrystalline uranium dioxide are first of their kind," says Desai. While predicting what happens to an entire piece of fuel, even over the course of a single day, is still far off, the researchers say understanding what happens to uranium dioxide at the molecular level will directly contribute to a full, multiphysics reactor simulation. "The insights we gain from this work will help us create more accurate models of material properties, a critical component in developing and licensing the next generation of nuclear reactors," says Desai.

A simulation of uranium dioxide shows how fractures can form in the material when it is stretched. Courtesy T. Desai.

Turbulence and Beyond

In addition to simulating fuel, the multiphysics team is developing models to understand turbulent coolant flows through the core of a reactor and how coolant transports heat away from the core. The solution will help simulate another coupled, chicken-and-egg physics problem - the relationship between coolant temperature and fission rate.

The bigger goal is to create a model that pulls together computational solutions to all the tricky reactor problems, from fuel damage and materials performance to coolant flow and neutronics. Creating a simulation that incorporates so many different physical processes will not be easy. "It's a great problem to work on," says computational physicist Dana Knoll, who heads up the multiphysics effort. "To get where we want to go, it's going to stretch the limits of our computational mathematics and well as the power of our computing." While it will take a number of years to achieve a working predictive nuclear reactor simulation, researchers say the payoffs, in efficiency and safety, are well worth the effort.

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